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Lisa Medley/DC/USEPA/US
12/29/2005 09:38 AM

To NCIC HPV@EPA
cc
bcc
Subject Fw: HPV Challenge Submission for CAS Number 101-14-4

Lisa Medley
OPPT/OSWER Docket - EPA HQ Docket Center
(Operated by ASRC Management Services)
1301 Constitution Ave NW Room B146 West
Washington DC 20460
202-566-0271 *fax 202-566-0282
----- Forwarded by Lisa Medley/DC/USEPA/US on 12/29/2005 09:38 AM -----

Wendy Koch <wendykoch@eponallc.com>
12/28/2005 09:15 AM

To NCIC OPPT@EPA, Rtk Chem@EPA
cc sheridan.diane@epa.gov', 'townsend.mark@epa.gov', Oscar Hernandez/DC/USEPA/US@EPA, '"Donald P. Gallo"' <dgallo@reinhartlaw.com>, '"Mike Kocak"' <mikek@cue-inc.com>, '"Mike Katz"' <mkatz@moldeddimensions.com>, '"Taylor, Alan - Middlebury, CT"' <Alan.Taylor@chemtura.com>
Subject HPV Challenge Submission for CAS Number 101-14-4

Dear Sir or Madam,
The MBOCA Consortium is a group of MBOCA manufacturers, distributors, suppliers and processors. On behalf of the MBOCA Consortium, I am submitting the MBOCA Consortium's test plan and robust summaries for CAS Number 101-14-4 (9th Collective Index Name: Benzenamine, 4,4'-methylenebis[2-chloro-) as part of our commitment under the HPV Challenge Program. If you have any questions regarding our commitment, please feel free to contact Don Gallo at 262-951-4555 or dgallo@reinhartlaw.com. You may also contact me at (860) 429-0038 or wendykoch@eponallc.com.

Wendy H Koch, PhD
Epona Associates, LLC
156 River Rd Studio 3
Willington CT 06279

tel 860 429 0038
fax 860 429 0151

TestPlanCASNo101144_Dec27_2005.pdf Appendix1&2CASNo101144_Dec27_2005.pdf

4,4'-Methylenebis-(2-Chlorobenzenamine)
(MOCA, MBOCA)
(CAS No. 101-14-4)
TEST PLAN

Submitted to the US Environmental Protection Agency

By

MBOCA Consortium

DATE: December 27, 2005

SUMMARY

The MBOCA Consortium has sponsored 4,4'-Methylenebis-(2- chlorobenzenamine) (MOCA, MBOCA; CAS No. 101-14-4) under the EPA's High Production Volume (HPV) Program. This document provides the Test Plan and summaries of existing data for this substance.

1.0 INTRODUCTION

The MBOCA Consortium has voluntarily committed to participate in the Environmental Protection Agency's (EPA) high production volume chemicals (HPV) challenge program, to assess the health and environmental effects, including selected physical chemical characteristics of 4,4'-Methylenebis-(2- chlorobenzenamine) (MOCA, MBOCA; CAS No. 101-14-4).

An evaluation of the available data and proposed test plan are included in this document. Robust summaries are attached in Appendix 1.

The objective of this test plan is to evaluate the available data and determine what additional data, if any, are needed to adequately characterize the physical properties, environmental fate, and human health and environmental hazards of MOCA. It is proposed that additional studies be conducted as shown in Table 1.

Table 1: PROPOSED TESTING FOR MOCA; CAS NO. 101-14-4

Endpoint	Data
Physical Chemical Properties	
Melting Point	A
Vapor Pressure	A
Boiling Point	A
Partition Coefficient	A
Water Solubility	A
Environmental Fate	
Hydrolysis	A
Photodegradation	A
Biodegradation	A
Environmental Transport	A
Ecotoxicity	
Acute Fish	A
Acute Daphnia	A
Acute Algae	A
Mammalian toxicity	
Acute Oral	A
Acute Dermal	A
Repeated Dose	A
Genotoxicity (*in vitro* -bacteria)	A
Genotoxicity (*in vivo*)	A
Reproductive/Developmental	Test (OECD 422)

A= Adequate data
Test = Testing proposed

2.0 POTENTIAL USE AND EXPOSURE

MOCA is used in the United States as a curing agent in manufacturing castable polyurethane products. During 1995, about two million pounds of the chemical were used in castable polyurethane processing. This MOCA was supplied by Japanese and

Taiwanese producers since no MOCA has been manufactured in the United States since 1979.

MOCA is an important chemical as adequate substitute curatives have not been found for certain MOCA cured polyurethane products. MOCA cured polyurethane produces a tough abrasion-resistant polymer not duplicated in polyurethane manufactured with other curatives. MOCA also provides unusual processing characteristics important to producing certain products.

The Polyurethane Manufacturers Association ("PMA") represents the castable polyurethane industry and has been involved with governmental agencies and non-governmental bodies regarding regulatory matters involving MOCA since 1973. MOCA has been classified as a "carcinogen" since the early 1970s. This classification is based upon test results with laboratory animals. The American Conference of Governmental Industrial Hygienists ("ACGIH") as recently as 1992 after reviewing existing information continued the classification of MOCA as a "Suspect Human Carcinogen."

Since the 1970s industry has developed an effective program to control employee exposure to the chemical and to monitor that exposure. Governmental agencies including the Occupation Safety & Health Administration ("OSHA") and the Environmental Protection Agency ("EPA") have been complimentary of this industry program (www.mocahome.org)

3.0 EVALUATION OF EXISTING DATA AND PROPOSED TESTING

The available data have been assessed (see Tables 2 through 5). Robust summaries are provided as Appendix 1.

Chemical/Physical Properties:

The melting point of MOCA is 102-107 °C (Aldrich, 2000-2001). This is in good agreement with the EPIWIN modeled value of 110 °C (The Merck Index, 1983). The boiling point is estimated to be 378.9 °C (SRC ,1988). The vapor pressure is 0.0000133 hPa (Smith and Woodward, 1983). The calculated partition coefficient is 3.61-3.9 (Leo, 1978). The water solubility of MOCA is 13.9 mg/L at 24 °C (Voorman and Penner, 1986). The EPIWIN modeling summary is provided in Appendix 2.

TABLE 2: PHYSICAL CHEMICAL PROPERTIES FOR MOCA; CAS NO. 101-14-4

Endpoint	Result
Melting Point	102-107 °C
Vapor Pressure	.0000133 hPa at 25 °C
Boiling Point	378.9 °C
Partition Coefficient	3.61-3.9
Water Solubility	13.9 mg/L at 24 °C

Recommendation: No additional testing is proposed.

Environmental Fate:

EPIWIN was used to predict the photodegradation and environmental distribution (see Appendix 2 for EPIWIN summary). The Overall OH Rate Constant is 77.5166 E-12 cm3/molecule-sec and the predicted half-life is 0.138 days (US EPA, 2003). Level III fugacity modeling indicates distribution to soil will predominate (US EPA, 2003). The hydrolysis of the sponsored substance is slow (USEPA, 1988). MOCA does not biodegrade (Chemicals Inspection and Testing Institute, 1992).

Recommendation: No further testing is proposed.

TABLE 3: ENVIRONMENTAL FATE DATA FOR MOCA; CAS NO. 101-14-4

Endpoint	Result
Hydrolysis	Half-life > 1 year
Photodegradation	Overall OH Rate Constant = 77.5166 E-12 cm3/molecule-sec Half-Life = 0.138 days
Biodegradation	0% after 28 days
Environmental Transport (Level III Fugacity modeling)	Air 9.87e-005 Water 15.5 Soil 82.1 Sediment 2.42

Aquatic Toxicity:

Acute aquatic toxicity data are available for fish, daphnia and algae for the sponsored substance. Although details of these studies are not readily available, the studies were conducted by Japanese MOE and these studies are widely accepted as valid. The 96 hour LC50 to fish (*Oryzias latipes*) was 0.61 mg/L (National Institute of Technology and Evaluation, Ministry of the Environment, 2001). The 48 hour LC50 for *Daphnia magna* is 0.92 mg/L (National Institute of Technology and Evaluation, Ministry of the Environment, 2001). In algae (*Selenastrum capricornutum*) the 48 hr ECr50 and 72 hr ECb50 are both > 1.9 mg/L. The 48 and 74 hour NOEC's are 1.4 and 0.74 mg/L, respectively (National Institute of Technology and Evaluation, Ministry of the Environment, 2001).

A 21 day reproduction study with *Daphnia magna* has been conducted by the Japanese MOE. The 21 day EC50 and NOEC are 0.052 and 0.0095 mg/L, respectively (National Institute of Technology and Evaluation, Ministry of the Environment, 2001).

TABLE 4: ENVIRONMENTAL EFFECTS DATA FOR MOCA; CAS NO. 101-14-4

Endpoint	Result
96 hr LC50 Fish (mg/L)	0.61
48 hr LC50 Daphnia (mg/L)	0.92
96 hr EC50 Algae (mg/L)	ECr50 >1.9 ECb50 >1.9
Chronic Daphnia (21 d EC50) (mg/L)	0.052

Recommendation: No additional testing is proposed.

Acute Mammalian Toxicity:

Acute oral and dermal studies have been conducted. The acute oral LD50 in rats is 1140 mg/kg (Lewis, 1996). The dermal LD50 in rabbits is greater than 5000 mg/kg (Lewis, 1996).

Recommendation: No additional testing is proposed.

Repeated Dose/ Reproductive/Developmental Toxicity:

Standard repeated dose toxicity studies have not been conducted with MOCA. However, extensive cancer studies have been conducted from which the toxicity of this substance can be described.

Rats were fed 12.5, 25 or 50 mg MOCA/kg/day on standard protein diet or 6.25, 12 or 25 mg MOCA/kg/day on low protein diet for 18 months (Kommineni et al., 1979). A dose-dependent increase in lung tumors was observed in rats fed 12.5, 25, or 50 mg/kg/day of MBOCA for 18 months; the incidence of lung tumors was 23%, 37%, and 70%, respectively (results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA; U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry). In contrast, the incidence of lung tumors in rats was lower if animals were fed MBOCA in a protein-deficient diet. In rats fed 6.25, 12, or 25 mg/kg/day of MBOCA in a low protein diet for 18 months, the incidences of lung tumors were 6%, 15%, and 26%, respectively, while no tumors were found in control animals. These numbers are less than half of the incidences reported for comparable doses of MBOCA given to rats fed a standard diet. MBOCA also induces liver tumors in rats. An increase in the incidence of hepatomas was found in rats fed 25 or 50 mg/kg/day of MBOCA in a standard protein diet for 18 months; the incidences were 4% and 36%, respectively. The effect of standard and low protein diets on the incidence of MBOCA-induced hepatocellular carcinomas was investigated in rats. In Sprague-Dawley rats fed 12.5 or 25 mg/kg/day of MBOCA in a standard protein diet for 18 months, the incidences of hepatocellular carcinomas were 3% and 4%, respectively; in rats fed the same amounts of MBOCA in a protein-deficient diet, the incidences were 0% and 18%, respectively. These results indicate that a protein-deficient diet did not reduce the MBOCA-induced incidence of hepatocellular carcinoma

in rats. A similar finding was made in male rats fed 25 mg/kg/day of MBOCA in a low protein diet for 18 months; the incidence of mammary tumors was 6%. When rats were fed a standard diet, the incidence of mammary adenocarcinoma was 28% at 50 mg/kg/day of MBOCA and 11% at 25 mg/kg/day. Zymbal's gland carcinomas were found in 12% of rats fed a low protein diet and in 7% of rats fed a standard-protein diet; both diets contained 25 mg/kg/day MBOCA. The results in rats fed MBOCA in low and standard protein diets indicate that there is a dose-related increase in the incidence of lung and mammary carcinomas, while the incidence of hepatocellular carcinoma is not dose-related. Other tumor types were also found after chronic oral administration of MBOCA. The incidence of hemangiosarcomas was 4% and 8% in rats fed 25 mg/kg/day of MBOCA in standard protein or low protein diets, respectively. The incidence of pituitary adenomas (including adenocarcinomas) in rats fed a standard protein diet was reduced, especially in animals treated with high doses of MBOCA. Rats fed 12.5, 25, or 50 mg/kg/day of MBOCA for 18 months had 36%, 25% (statistically significant), and 4% (statistically significant) incidences of pituitary adenomas, respectively. The incidence of pituitary adenomas in the control group was 42%. MBOCA had an effect on the incidence of pituitary tumors in rats fed a low protein diet: the incidences were 16%, 12% (statistically significant), and 20% in animals fed 6.25, 12.5, and 25 mg/kg/day, respectively. In the control group, the incidence of pituitary adenomas was 23%.

Rats were fed 50 mg MBOCA/kg/day in standard protein diet or 50 mg MBOCA/kg/day in low protein diet for two years (Stula et al., 1975). The effect of standard and low protein diets on the incidence of MBOCA-induced lung adenocarcinomas was investigated in rats: the incidence of lung tumors in rats fed a protein-deficient diet was roughly one-half of that observed in rats fed a standard protein diet (results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA; U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry). The effect of standard and low-protein diets on the incidence of MBOCA-induced hepatocellular carcinomas was investigated in rats. The results are inconclusive. When male rats were fed 50 mg/kg/day of MBOCA for 2 years, the incidences of hepatocellular carcinomas were 7% in rats fed a standard-protein diet and 52% in rats fed a low protein diet. This observation, that the protein-deficient diet accentuates the carcinogenic effects of MBOCA, was not seen in female rats that had 7% and 5% hepatocellular carcinomas when fed standard-protein and low-protein diets, respectively. A statistically significant increase of malignant mammary tumors was found in female Charles River rats fed 50 mg/kg/day of MBOCA in a low-protein diet for 2 years. A statistically significant decrease in pituitary tumors was also observed in female, but not male, rats.

Male rats were fed 25 or 50 mg MBOCA/kg/day in a standard protein diet for18 months (Russfield et al., 1975). Lung adenocarcinomas were reported in 1/22 and 1/19 animals, respectively, although this finding was not statistically significant (results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA; U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry). In addition, 3 of 22 and 4 of 19 rats receiving 25 or 50 mg/kg/day of MBOCA, respectively, developed adenomatosis, which is a

preneoplastic lesion. MBOCA also induced liver tumors in rats. An increase in the incidence of hepatomas was found; the incidences were 5% and 21%, respectively (not statistically significant). A limitation of this study is the small number of animals on which the tumor incidence was based.

Mice were fed 130 or 260 mg/kg/day for 18 months, and followed for an additional 6 months post-exposure (Russfield et al., 1975). MBOCA induced liver tumors in mice. There was a significantly increased incidence of hepatomas, 43% in the 130-mg/kg/day group and 50% in the 260-mg/kg/day group was reported (results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA; U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry). The incidence of hepatomas in treated random-bred male albino mice was not significantly different from that in controls. These results indicate that in mice there is a gender difference regarding MBOCA-induced hepatomas; female mice are affected, and male mice are not affected. Vascular tumors (generally subcutaneous hemangiomas and hemangiosarcomas) were reported in randomly bred male albino mice fed 130 or 260 mg/kg/day of MBOCA for 18 months; the incidences were 23% and 40%, respectively. In female mice, vascular tumors (43%) were present only in the group treated with the high dose of 260 mg/kg/day of MBOCA.

Rats were fed 54 mg MBOCA/kg/day in a low protein diet for 500 days (Grundmann and Steinhoff, 1970). 32% of males and 12% of females developed lung tumors. Liver cancer was present in 88% of males and 72% of females (results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA; U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry).

Beagle dogs were fed 10 mg MBOCA /kg/day for 9 years (Stula et al., 1977). One beagle died approximately 3.4 years of pyelonephritis unassociated with MBOCA exposure. Of the five surviving dogs, three developed papillary transitional cell carcinomas of the urinary bladder; and one dog had a combined urethral adenocarcinoma and transitional cell carcinoma (results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA; U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry). Despite the small number of animals used, this study demonstrates that ingestion of MBOCA over 9 years was associated with the appearance of carcinomas of the urinary bladder and urethra in dogs.

Male rats were fed diets containing 0, 500 or 1000 mg/kg of diet MOCA as the hydrochloride (97% pure) for 18 months (IARC, 1993). All surviving animals were killed 24 months after the start of the study; about 55% of the control and treated animals were still alive at 20-22 months. The effective numbers were: 22 control, 22 low-dose and 19 high-dose animals. Hepatomas occurred in 0/22 control, 1/22 low-dose and 4/19 high-dose rats.

Groups of rats were fed 0 (control) or 1000 mg/kg of diet MOCA (approximately 95% pure) in a standard diet (23% protein) for life (IARC, 1993). The average duration of the experiment was 560 days (80 weeks) for treated males, 548 days (78 weeks) for treated females, 564 days (80 weeks) for male controls and 628 days (89 weeks) for female controls. Six animals from each group were sacrificed at one year for interim evaluation. Lung adenocarcinomas occurred in 21/44 ($p < 0.05$, 2 test) treated males and 27/44 ($p < 0.05$, 2 test) treated females. An additional squamous-cell carcinoma of the lung was observed in one treated male and one treated female. No lung tumor was observed among control animals. Lung adenomatosis, considered to be a preneoplastic lesion, developed in 14/44 treated males and 11/44 treated females and in 1/44 male controls and 1/44 female controls ($p < 0.05$). Pleural mesotheliomas occurred in 4/44 treated males and 2/44 treated females; no such tumor was observed among controls. Hepatocellular adenomas and hepatocellular carcinomas occurred in 3/44 and 3/44 treated males and in 2/44 and 3/44 treated females, respectively, but not in controls. Ingestion of MOCA resulted in a lower incidence of pituitary tumors in treated females than in controls (1/44 versus 12/44).

No reproductive toxicity or developmental studies have been conducted with MOCA.

Recommendation: A combined repeat dose with developmental and reproductive screen (OECD 422) is proposed to fulfill a standard repeat dose toxicity endpoint as well as reproductive toxicity and developmental effects.

Mutagenicity Assays:

In vitro testing indicates that MOCA is mutagenic in the *Salmonella typhimurium* /mammalian microsome mutagenesis assay and that the mutagenic effect requires exogenous metabolic activation (Ames et al., 1975; ATSDR, 1994; Baker and Bonin, 1981; Butler et al., 1989; Chen et al., 1989; Cocker et al., 1985; 1986; Dunkel et al., 1984; Hesbert et al., 1985; Kuslikis et al., 1991; MacDonald, 1981; Martire et al., 1981; Matsushima et al., 1981; McCann et al., 1975; Messerly et al., 1987; Morton et al., 1988; Rao et al., 1982; and Walker, 1984). In vivo animal studies provide direct and indirect evidence that MOCA is a mutagen (ATSDR, 1994; Caspary et al., 1988; Cheever et al., 1990; Daniel and Dehnel, 1981; Dunkel et al., 1984; Galloway et al., 1985; Katz et al., 1981; Kugler-Stegmeier et al., 1989; Martin and McDermid, 1981; McQueen et al., 1981; 1983; 1987; Mori et al., 1988; Myhr and Caspary, 1988; Perry and Thomson, 1981; Salamone et al., 1981; Styles, 1981; Traul et al., 1981; Tsuchimoto and Matter, 1981; Vogel et al., 1981; and Williams et al., 1982).

Recommendation: No additional testing is proposed.

TABLE 5: MAMMALIAN TOXICITY DATA FOR MOCA; CAS NO. 101-14-4

Endpoint	Result
Acute Oral LD50 (mg/kg)	1140 (rat)
Acute Dermal LD50 (mg/kg)	>5000 (rabbit)
Repeated Dose	NOAEL (18 mo dietary, standard protein diet, cancer, rat) = 6.25 % LOAEL (18 mo dietary, low protein diet, cancer, rat) = 12.5 % LOAEL (2 yr dietary, standard or low protein diet, systemic toxicity, rat) = 50 mg/kg/d LOAEL (2 yr dietary, standard or low protein diet, cancer, rat) = 50 mg/kg/d LOAEL (18 mo dietary, standard protein diet, systemic toxicity, rat) = 25 mg/kg/d LOAEL (18 mo dietary, cancer, rat) = 25 mg/kg/d LOAEL (18 mo dietary, cancer, mouse) = 130 mg/kg/d LOAEL (500 d dietary, low protein diet cancer, rat) = 54 mg/kg/d LOAEL (9 yr dietary, systemic toxicity, dog) = 10 mg/kg/d LOAEL (9 yr dietary, cancer, dog) = 10 mg/kg/d LOAEL (18 mo dietary, cancer, rat) = 500 mg/kg/d LOAEL (lifetime dietary, standard protein diet, cancer, rat) = 1000 mg/kg/d
Genotoxicity (*in vitro* - bacteria)	Positive
Genotoxicity (*in vivo*)	Positive
Reproductive/Developmental	No data available

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APPENDIX 1
ROBUST SUMMARIES

I U C L I D

Data Set

Existing Chemical	:	ID: 101144
Producer related part		
Company	:	Epona Associates, LLC
Creation date	:	19.12.2005
Substance related part		
Company	:	Epona Associates, LLC
Creation date	:	19.12.2005
Status	:	
Memo	:	MOCA
Printing date	:	22.12.2005
Revision date	:	
Date of last update	:	22.12.2005
Number of pages	:	19
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	= 102 - 107 °C
Sublimation	:	
Method	:	other
Year	:	2000
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Data are taken from a secondary literature source (handbook)
Flag	:	Critical study for SIDS endpoint

19.12.2005 (2)

Value	:	= 110 °C
Sublimation	:	
Method	:	other
Year	:	1983
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(1) valid without restriction Data were obtained by modeling, SRC recommended value

19.12.2005 (56)

2.2 BOILING POINT

Value	:	= 378.9 °C at
Decomposition	:	
Method	:	other: calculation
Year	:	1988
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Data were obtained by modeling, estimated by PCCHEM-PCGEMS, SRC recommended value
Flag	:	Critical study for SIDS endpoint

19.12.2005 (51)

2.4 VAPOUR PRESSURE

Value	:	= .0000133 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	1983
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor pressure = 1.0 x 10E-5 mm Hg at 25 deg C
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data
Flag	:	Critical study for SIDS endpoint

21.12.2005 (50)

Value	:	< 0 hPa at 25 °C

Decomposition	:	
Method	:	other (calculated)
Year	:	1988
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor pressure = 1.32E-8 mm Hg at 25C Calc
Reliability	:	(2) valid with restrictions Data were obtained by modeling, estimated by PCCHEM-PCGEMS, SRC recommended value
19.12.2005		(51)
Value	:	< 0 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2003
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor pressure = 2.86X10-7 mm Hg @ 25 deg C Calc
Reliability	:	(2) valid with restrictions Data were obtained by modeling
19.12.2005		(59)
Value	:	= .0000173 hPa at 60 °C
Decomposition	:	
Method	:	
Year	:	1981
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor pressure = 1.3 x 10E-5 mm Hg at 60 deg C
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data
21.12.2005		(43)
Value	:	= .00173 hPa at 60 °C
Decomposition	:	
Method	:	other (measured)
Year	:	2001
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor pressure = 1.3X10-3 torr @ 60 deg C
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data
21.12.2005		(1)
Value	:	= .0000466 hPa at 100 °C
Decomposition	:	
Method	:	
Year	:	1983
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor pressure = 3.5 x 10E-5 mm Hg at 100 deg C
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data
20.12.2005		(50)
Value	:	= .0000719 hPa at 120 °C
Decomposition	:	

Method	:	
Year	:	1981
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Vapor pressure = 5.4 x 10E-5 mm Hg at 120 deg C
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data

20.12.2005 (43)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 3.61 - 3.9 at °C
pH value	:	-
Method	:	other (calculated)
Year	:	1978
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions EPA source document
Flag	:	Critical study for SIDS endpoint

19.12.2005 (27)

Partition coefficient	:	octanol-water
Log pow	:	= 3.94 at °C
pH value	:	
Method	:	other (calculated)
Year	:	1988
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Data were obtained by modeling, estimated by PCCHEM-PCGEMS, SRC recommended value

19.12.2005 (51)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 13.9 mg/l at 24 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	1986
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data
Flag	:	Critical study for SIDS endpoint

19.12.2005 (61)

Solubility in	:	Water
Value	:	= 8.684 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Water Solubility Estimate from Log Kow (WSKOW v1.41): Water Solubility at 25 deg C (mg/L): 8.684 log Kow used: 3.91 (expkow database) no-melting pt equation used
Reliability	:	(2) valid with restrictions Data were obtained by modeling

20.12.2005 (59)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	
Rate constant	:	= .0000000000775166 cm³/(molecule*sec)
Degradation	:	= 50 % after .1 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 77.5166 E-12 cm3/molecule-sec Half-Life = 0.138 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 1.656 Hrs Ozone Reaction: No Ozone Reaction Estimation
Reliability	:	(2) valid with restrictions Data were obtained by modeling
Flag	:	Critical study for SIDS endpoint

21.12.2005 (59)

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	500000 molecule/cm³
Rate constant	:	= .0000000000775 cm³/(molecule*sec)
Degradation	:	= 50 % after 5 hour(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	1993
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	t1/2 = 5 hours ; rate constant = 7.75X10-11 cu cm/molecule-sec at 25 deg C
Reliability	:	(2) valid with restrictions Data were obtained by modeling

20.12.2005 (38)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	at °C

Deg. product	:	
Method	:	other: measurement
Year	:	1988
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions EPA source document
Flag	:	Critical study for SIDS endpoint

19.12.2005 (17)

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	> 800 year at 25 °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other
Year	:	1989
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	4,4'-Methylenebis(2-chloroaniline) is not expected to undergo hydrolysis based on a hydrolysis half-life of greater than 800 years at pH 7 and 25 deg C.
Reliability	:	(2) valid with restrictions EPA source document

19.12.2005 (16)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other
Year	:	2005
Result	:	Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	9.87e-005	3.31	1000
Water	15.5	1.44e+003	1000
Soil	82.1	1.44e+003	1000
Sediment	2.42	5.76e+003	0

Persistence Time: 1.59e+003 hr

Reliability	:	(2) valid with restrictions Data were obtained by modeling
Flag	:	Critical study for SIDS endpoint

21.12.2005 (59)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge

Concentration	:	100 mg/l related to Test substance related to
Contact time	:	28 day(s)
Degradation	:	= 0 (±) % after 28 day(s)
Result	:	under test conditions no biodegradation observed
Deg. product	:	
Method	:	other
Year	:	1992
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	4,4'-Methylenebis(2-chloroaniline) is not expected to undergo biodegradation based on a screening test. 4,4'-Methylenebis(2-chloroaniline), present at 100 mg/liter, reached 0% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/liter and the Japanese MITI test.
Reliability	:	(2) valid with restrictions Japanese CITI studies are widely accepted as valid
Flag	:	Critical study for SIDS endpoint

20.12.2005 (10)

Type	:	aerobic
Inoculum	:	activated sludge
Concentration	:	2 mg/l related to Test substance related to
Contact time	:	
Degradation	:	= 0 (±) % after 42 day(s)
Result	:	
Deg. product	:	
Method	:	other
Year	:	1979
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4

Method :

STATIC SYSTEM:
BSA -- Biodegrades slow with acclimation
Rate: 10; 0; 0; 3; 1; 7; 6
Rate Units: % DEGRADATION
Oxygen Condition: AEROBIC
Analysis Method: GC
Incubation Time [Days]: 7
Test Chemical Conc. [ppm]: 2
Acclimation Period [Days]: 7; 14; 21; 28; 35; 42
Dissolved Organic Carbon: YEAST EXTRACT
Microbial Population: 10 (%)
Inoculum: ACTIVATED SLUDGE
Temperature [degrees C]: 25
Remarks: FLASKS SUBCULTURED FROM PREVIOUS WEEK

CONTINUOUS FEED SYSTEM
BFA -- Biodegrades fast with acclimation
Rate: 96; 96; 100; 94; 77; 100
Rate Units: % DEGRADATION
Oxygen Condition: AEROBIC
Continuous/Semi-Continuous Activated Sludge: c
Analysis Method: GC
Retention Time [Days]: 24
Test Chemical Conc. [ppm]: 2
Acclimation Period [Days]: 7; 14; 21; 28; 35; 42
Inoculum: ACTIVATED SLUDGE
Temperature [degrees C]: 25

Result : 4,4'-Methylenebis(2-chloroaniline) was not degraded after 6 weeks in a

static system in which 2 mg/l of the compound was seeded with sludge, incubated for 7 days, and the process repeated using cultures from the original system. However, when 4,4'-methylenebis(2-chloroaniline) containing water to a continuous feed activated sludge reactor, 96% of the chemical in the water was removed in 24 hours after 1 week of operation.

Reliability : (2) valid with restrictions
EPA source document

20.12.2005

(18)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	Oryzias latipes (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= .61
Method	:	other
Year	:	2001
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Japanese MOE studies are widely accepted as valid
Flag	:	Critical study for SIDS endpoint

21.12.2005 (42)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= .92
Method	:	other
Year	:	2001
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Japanese MOE studies are widely accepted as valid
Flag	:	Critical study for SIDS endpoint

21.12.2005 (42)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: growth rate and biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
Method	:	other
Year	:	2001
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	Growth rate: 48 hr ECr50 > 1.9 mg/L; 48 hr NOEC = 1.4 Biomass: 72 hr ECb50 > 1.9 mg/L; 72 hr NOEC = 0.74
Reliability	:	(2) valid with restrictions Japanese MOE studies are widely accepted as valid
Flag	:	Critical study for SIDS endpoint

21.12.2005 (42)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1140 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1996
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data
Flag	:	Critical study for SIDS endpoint

19.12.2005 (28)

Type	:	LD0
Value	:	= 640 mg/kg bw
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1996
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data

19.12.2005 (28)

Type	:	other
Value	:	
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	2000
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	In mice, poisoning is accompanied by adynamia, apathy, loss of appetite. Death occurs in 3 days. Manifestations of the toxic action in rats are not very pronounced and death occurs in 2 days. The LOEL for methemoglobinemia formation appears to be 83 mg/kg bw. Gross pathology examination revealed distention of the stomach and intestine, traces of blood in the urinary bladder, and pleural effusion in the thorax. Histology examination detected fine-drop adiposis of the liver, tiny foci of inflammatory infiltration, and circulatory disturbances in the visceral organs.
Reliability	:	(2) valid with restrictions

Source is peer-reviewed published data

20.12.2005 (49)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 5000 - mg/kg bw
Species	:	rabbit
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	other
Year	:	1996
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Source is peer-reviewed published data

21.12.2005 (28)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Bacterial reverse mutation assay
System of testing	:	Salmonella typhimurium TA98 and TA100; Escherichia coli WP2uvrA
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	with
Result	:	positive
Method	:	other
Year	:	1994
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry
Result	:	In vitro testing has provided clear and convincing evidence that MBOCA is mutagenic in the Salmonella typhimurium/mammalian microsome mutagenesis assay and that the mutagenic effect requires exogenous metabolic activation (Baker and Bonin 1981; Cocker et al. 1985; Dunkel et al. 1984; MacDonald 1981; Martire et al. 1981; McCann et al. 1975; Messerly et al. 1987; Rao et al. 1982). Although not all investigators used each tester strain, the general result is that MBOCA is mutagenic only in strains TA98 and TA100, at 250 µg/plate, with some inconsistency regarding strain TA98. MBOCA and its metabolites are not mutagenic in S.

typhimurium strains TA1535, TA1537, or TA1538. This suggests that the mutagenic effect of MBOCA metabolites in some bacteria is dependent on the plasmid pKM101; strains TA98 and TA100 contain this plasmid, but strains TA1535, TA1537, and TA1538 do not (Ames et al. 1975). This hypothesis is supported by the finding that S9-activated MBOCA is mutagenic in Escherichia coli strain WP2uvrA only in the presence of the plasmid pKM101 (Matsushima et al. 1981). The plasmid carries genes involved in an "errorprone" DNA repair system that introduces mutations as it removes DNA damage (Walker 1984). S9 derived from dog and human liver could activate MBOCA to a form mutagenic to strain TA100 but only in a protocol using a fluctuation assay (Cocker et al. 1985).

Most of MBOCA's mutagenic activity appears to be due to the N-hydroxy metabolite, which caused dose-dependent increases in mutations of S. typhimurium strains TA100 and TA98 in a pre-incubation assay using nonactivated doses of =5 µg/plate (Kuslikis et al. 1991). This metabolite is produced by several species, including dogs and humans (Butler et al. 1989; Chen et al. 1989; Morton et al. 1988). The mononitroso derivative appears to be direct-acting mutagen but is much less potent, causing a statistically significant revertant increase in the pre-incubation assay at the highest tested nontoxic dose (50 µg/plate). Neither the o-hydroxy nor the dinitroso derivatives were direct-acting mutagens at up to 50 or 500 µg/plate, respectively. Neither chemical was tested to cytotoxic levels (Kuslikis et al. 1991). N-acetylation is a deactivating step. Neither n-acetyl nor N,N-diacetyl derivatives were mutagenic in S. typhimurium in the absence of activation (Hesbert et al. 1985). In the presence of S9 activation, the mutagenic activity of the acetylated derivatives is less than that of the parent compound (Cocker et al. 1986; Hesbert et al. 1985).

Conclusion : In vitro testing has provided clear and convincing evidence that MBOCA is mutagenic in the Salmonella typhimurium/mammalian microsome mutagenesis assay and that the mutagenic effect requires exogenous metabolic activation

Reliability : (2) valid with restrictions
Source is peer-reviewed published data

Flag : Critical study for SIDS endpoint

21.12.2005 (3) (4) (5) (6) (11) (12) (13) (15) (21) (26) (29) (31) (32) (33) (37) (40) (45) (62)

Type : DNA damage and repair assay
System of testing :
Test concentration :
Cycotoxic concentr. :
Metabolic activation :
Result : positive
Method : other
Year : 1994
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Remark : Results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

Result : DNA adducts have been found following oral (Cheever et al. 1990; Kugler-Steigmeier et al. 1989; Segerback and Kadlubar 1992) and dermal (Cheever et al. 1990) administration of radiolabeled MBOCA to rats, following the incubation of radiolabeled MBOCA with explants of dog and human bladder urothelium (transitional cell epithelium) (Stoner et al. 1988) and incubation of rat DNA and radiolabeled N-hydroxy-MBOCA (Segerback and Kadlubar 1992). The level of binding increased with dose, but the increase was not linear. Considerable individual variation in binding levels, varying over at least a 10-fold range, was found in both dogs and humans. At least six adducts were found in dog bladder epithelium; four adducts

were found in human bladder epithelium, three of which appeared to be the same as those found in dogs. DNA adduct formation in dog bladder tissue is of particular note, since MBOCA has been found to cause bladder tumors in dogs (Stula et al. 1977).

Reliability : (2) valid with restrictions
Source is peer-reviewed published data

Flag : Critical study for SIDS endpoint
20.12.2005

(4) (8) (25) (48) (52) (53)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	other
Species	:	
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	positive
Method	:	other
Year	:	1994
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Remark : Results excerpted from ATSDR (1994) Toxicological Profile for 4,4'-Methylene-bis(2-chloroaniline) MBOCA. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry

Result : In vivo animal studies provide direct and indirect evidence that MBOCA is a mutagen; MBOCA metabolites were bound to DNA following oral (Cheever et al. 1990; Kugler-Steigmeier et al. 1989) or dermal (Cheever et al. 1990) exposure in rats. Small increases in the SLRL values were observed in D. melanogaster adults fed a 7.5millimolar MBOCA solution for 3 days (Vogel et al. 1981).

MBOCA induced gene mutations at the thymidine kinase (TK) locus in mouse lymphoma cells (Caspary et al. 1988; Myhr and Caspary 1988). Unscheduled DNA synthesis (UDS) was induced in HeLa cells (Martin and McDermid 1981), in rat primary hepatocytes at >10 µmol (McQueen et al. 1981; Mori et al. 1988; Williams et al. 1982) and in hamster (McQueen et al. 1981) and rabbit (McQueen and Williams 1987) hepatocytes. The concentration that tested positive in the mouse was 50 µmol (McQueen et al. 1981). Sensitivity to MBOCA showed species-specific variations: rat > mouse > hamster > rabbit (McQueen et al. 1981, 1983). Because hepatocytes have their own metabolic activation systems, no exogenous metabolic activation is needed. In assays using attachment independence as an end point, MBOCA, at concentrations near the LC50, transformed baby hamster kidney (Daniel and Dehnel 1981; Styles 1981), rat embryo (Dunkel et al. 1981; Traul et al. 1981), and Balb/3T3 cells (Dunkel et al. 1981).

Transformation assays have not been evaluated as thoroughly as some other genotoxicity assays. In an interlaboratory comparison, one laboratory found equivocal evidence that nonactivated MBOCA induced sister chromatid exchange in Chinese hamster ovary cells at a dose of 5.0 µg/mL. The response is considered equivocal because the dose-response curve was inconsistent. The result was not confirmed by the second laboratory. In the presence of S9 activation, positive results were obtained by one laboratory at 50 µg/mL. The other laboratory observed the beginning of a dose-response curve, but the high-dose (30 µg/mL) results

did not meet the testing laboratory's criterion for a positive response. In a chromosome aberration assay testing activated and nonactivated concentrations up to 5 and 30 µg/mL, respectively, neither laboratory found a positive result (Galloway et al. 1985). Another study (Perry and Thomson 1981) found no evidence of sister chromatid exchange at up to cytotoxic doses (100 µg/mL), but no doses were tested in the probable sensitive range (>10 and <100 µg/mL). Thus, MBOCA is clastogenic in some systems but not others.

In another study, MBOCA was classified as a clastogen on the basis of results from an in vivo micronucleus bone marrow assay (Katz et al. 1981). Evaluations using a two-phase micronucleus assay and intraperitoneal dosing of B6C3F1 hybrid mice were incomplete, but the results suggested that MBOCA is an in viva clastogen at doses of >32 mg/kg (Salamone et al. 1981) or 50% of the 1 LD50 (Katz et al. 1981). Results were inconclusive because of toxicity during the first phase of testing in which mice were dosed at 0 and 24 hours with 80% of the LD50 (51 mg/kg), and results were evaluated at 48 hours. In the second phase of testing, mice were dosed with 32 or 51 mg/kg and sampled 48 hours later, or in a separate test, dosed with 32 or 48 mg/kg and sampled 36 hours later. Results were negative at 32 mg/kg when sampled at 48 hours but positive at the same dose in a separate assay when sampled at 36 hours. Results were positive at the higher dose for both sampling times. Multiple sampling times were not performed in any assay (Salamone et al. 1981). In another study, results in the micronucleus test were negative at doses up to 50% of the LD50 (32 mg/kg) using CD-1 mice (dosing was done intraperitoneally at 0 and 24 hours and sampling at 30 hours) (Tsuchimoto and Matter 1981).

Conclusion : n vivo animal studies provide direct and indirect evidence that MBOCA is a mutagen.

Reliability : (2) valid with restrictions
Source is peer-reviewed published data

Flag : Critical study for SIDS endpoint
21.12.2005 (4) (7) (8) (14) (15) (19) (23) (25) (30) (34) (35) (36) (39) (41) (44) (47) (55) (57) (58) (60) (63)

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

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APPENDIX 2
EPIWIN RESULTS

```
SMILES : Nc(c(cc(cl)Cc(ccc(N)c2CL)c2)CL)cl
CHEM   : Benzenamine, 4,4'-methylenebis 2-chloro-
CAS NUM: 000101-14-4
MOL FOR: C13 H12 CL2 N2
MOL WT : 267.16
------------------------------ EPI SUMMARY (v3.11) -------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   ------
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   ------
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   ------

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.67 estimate) =  3.47
    Log Kow (Exper. database match) =  3.91
       Exper. Ref:  Chem Inspect Test Inst (1992)

 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.41):
    Boiling Pt (deg C):  404.79  (Adapted Stein & Brown method)
    Melting Pt (deg C):  156.63  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  3.93E-006  (Modified Grain method)
    MP  (exp database):  110 deg C
    BP  (exp database):  378.9 deg C

 Water Solubility Estimate from Log Kow (WSKOW v1.41):
    Water Solubility at 25 deg C (mg/L):  8.684
       log Kow used: 3.91 (expkow database)
       no-melting pt equation used
     Water Sol (Exper. database match) =  13.9 mg/L (24 deg C)
        Exper. Ref:  VOORMAN,R & PENNER,D (1986A)

 Water Sol Estimate from Fragments:
    Wat Sol (v1.01 est) =  4.5958 mg/L
    Wat Sol (Exper. database match) =  13.90
       Exper. Ref:  VOORMAN,R & PENNER,D (1986A)

 ECOSAR Class Program (ECOSAR v0.99g):
    Class(es) found:
       Aromatic Amines

 Henrys Law Constant (25 deg C) [HENRYWIN v3.10]:
   Bond Method :   3.29E-011  atm-m3/mole
   Group Method:   1.14E-011  atm-m3/mole
 Henrys LC [VP/WSol estimate using EPI values]:  1.591E-007 atm-m3/mole

 Probability of Rapid Biodegradation (BIOWIN v4.01):
    Linear Model         :  -0.1573
    Non-Linear Model     :   0.0003
 Expert Survey Biodegradation Results:
    Ultimate Survey Model:   1.8508  (months      )
    Primary Survey Model :   2.8463  (weeks       )
 Readily Biodegradable Probability (MITI Model):
    Linear Model         :  -0.3921
    Non-Linear Model     :   0.0006
```

```
Atmospheric Oxidation (25 deg C) [AopWin v1.91]:
  Hydroxyl Radicals Reaction:
     OVERALL OH Rate Constant =  77.5166 E-12 cm3/molecule-sec
     Half-Life =     0.138 Days (12-hr day; 1.5E6 OH/cm3)
     Half-Life =     1.656 Hrs
  Ozone Reaction:
     No Ozone Reaction Estimation

Soil Adsorption Coefficient (PCKOCWIN v1.66):
     Koc    :  1.353E+004
     Log Koc:  4.131

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]:
   Rate constants can NOT be estimated for this structure!

BCF Estimate from Log Kow (BCFWIN v2.15):
   Log BCF =  2.311  (BCF = 204.5)
      log Kow used: 3.91 (expkow database)

Volatilization from Water:
   Henry LC:  1.14E-011 atm-m3/mole  (estimated by Group SAR Method)
   Half-Life from Model River: 8.394E+007  hours   (3.498E+006 days)
   Half-Life from Model Lake : 9.158E+008  hours   (3.816E+007 days)

Removal In Wastewater Treatment (recommended maximum 99%):
   Total removal:              26.13  percent
   Total biodegradation:        0.29  percent
   Total sludge adsorption:    25.84  percent
   Total to Air:                0.00  percent

Level III Fugacity Model:
          Mass Amount    Half-Life    Emissions
           (percent)        (hr)        (kg/hr)
  Air       9.87e-005      3.31          1000
  Water     15.5           1.44e+003     1000
  Soil      82.1           1.44e+003     1000
  Sediment  2.42           5.76e+003     0
    Persistence Time: 1.59e+003 hr
```
